Combustion Research Facility News

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LIF Images Show How Fuel Temperature and Ambient Cylinder Pressure Affect Spray Morphology in SIDI Gasoline Engines

Researchers at the CRF are investigating the fuel-air mixing process in spark-ignition direct-injection (SIDI) engines, which are of great interest because they offer significant potential for increasing the fuel economy of gasoline engines. Investigations are being carried out in two engine laboratories, one of which houses an optical engine with a vertical fuel injector mounted centrally above a flat piston (Figure 1). The simplified geometry in this central-injector engine optimizes optical access and facilitates studies of in-cylinder processes such as fuel injection, fuel mixing, and fuel impingement on walls.

In an SIDI engine, fuel injection can occur over a wide range of crank positions during the intake or compression strokes. As a result, ambient cylinder pressure and temperature at the time of injection vary widely. In addition, since the fuel injector is mounted in the engine head, the fuel warms up as the engine warms up. To understand the effect of these parameters on fuel sprays, CRF researchers Richard Steeper and Eric Stevens, working under the auspices of DOE's Office of Transportation Technologies and with the guidance of the big three U. S. automobile manufacturers, have recorded laser-induced fluorescence (LIF) images of gasoline sprays during direct injection in the SIDI engine.

The matrix of planar LIF images in Figure 2 illustrates how ambient cylinder pressure and fuel temperature can influence spray morphology. In each row, the spray images were recorded at the same ambient cylinder pressure but at increasing fuel temperatures (30 to 90 °C). The upper left image shows the classic hollow-cone spray produced by a high-pressure swirl injector at low ambient pressure and low fuel temperature. But as fuel temperature increases (left to right in Figure 2), the cone becomes progressively filled. A common explanation for this effect is that the hotter fuel produces smaller droplets (faster evaporation) that are more efficiently transported toward the low-pressure region along the spray axis. At the highest temperature (top right image), a plug of fuel has formed on the centerline causing an increase in penetration. In fact, the experiments have shown that while piston wetting can be avoided during cold-fuel injection, extensive wetting occurs for fuel temperatures of 90 °C. In each column of Figure 2, the ambient pressure at the time of injection increases from 0.5 to 1.0 to 2.0 bar. These sequences reveal the expected trend of reduced penetration as density and drag increase.

Figure 1. The optically accessible spark-ignited direct–injected (SIDI) research engine used for visualization of the fuel-air mixing process. Planar laser-induced fluorescence has been used to reveal the morphology of in-cylinder fuel sprays.

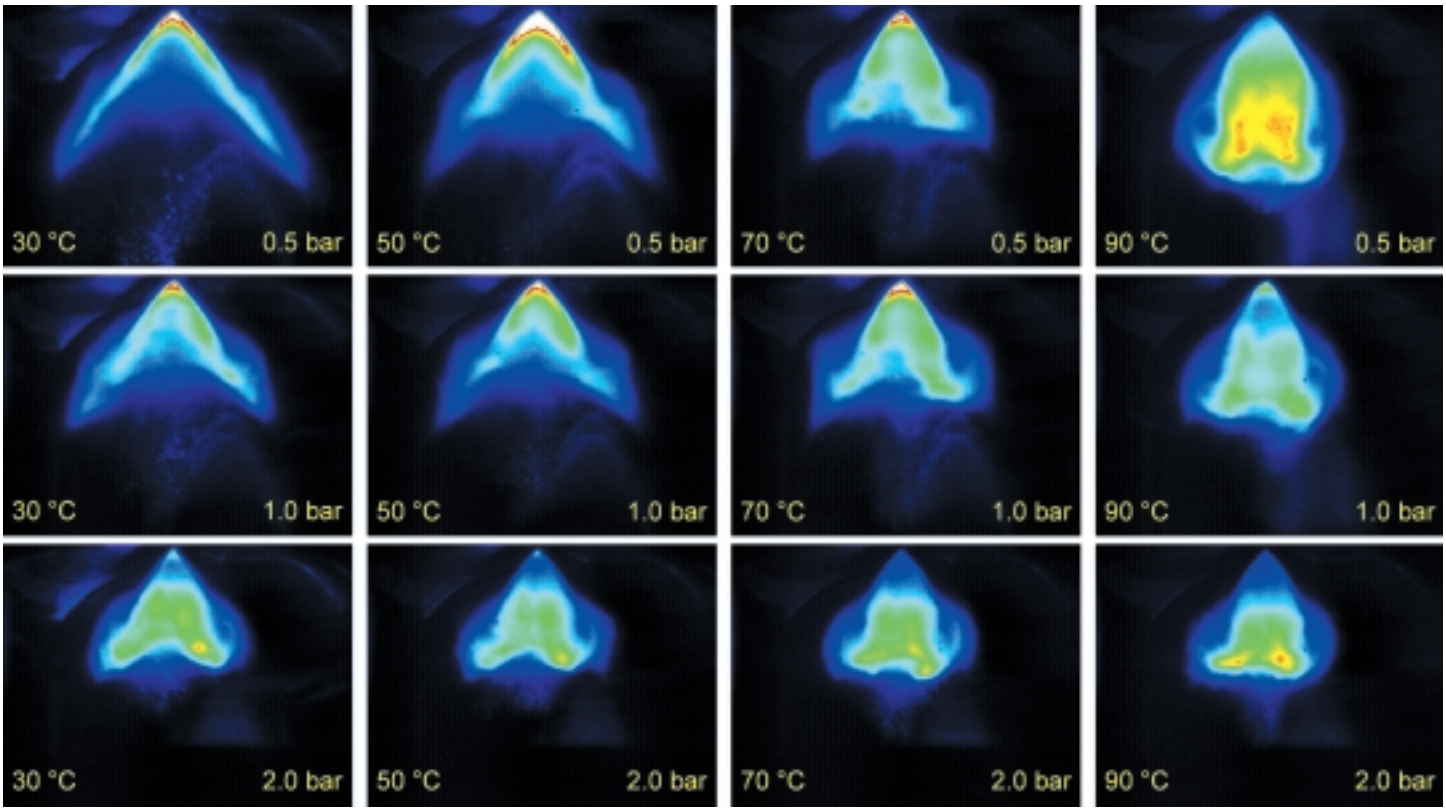
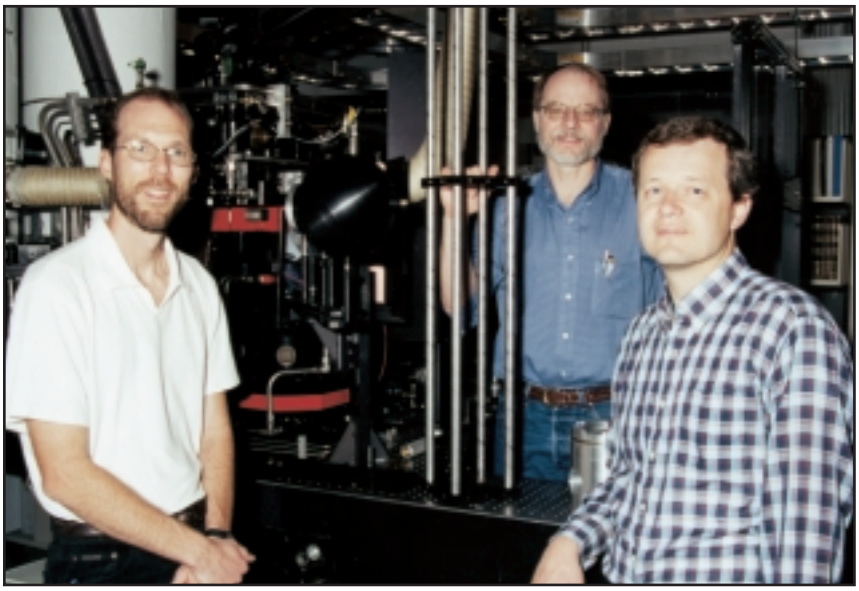


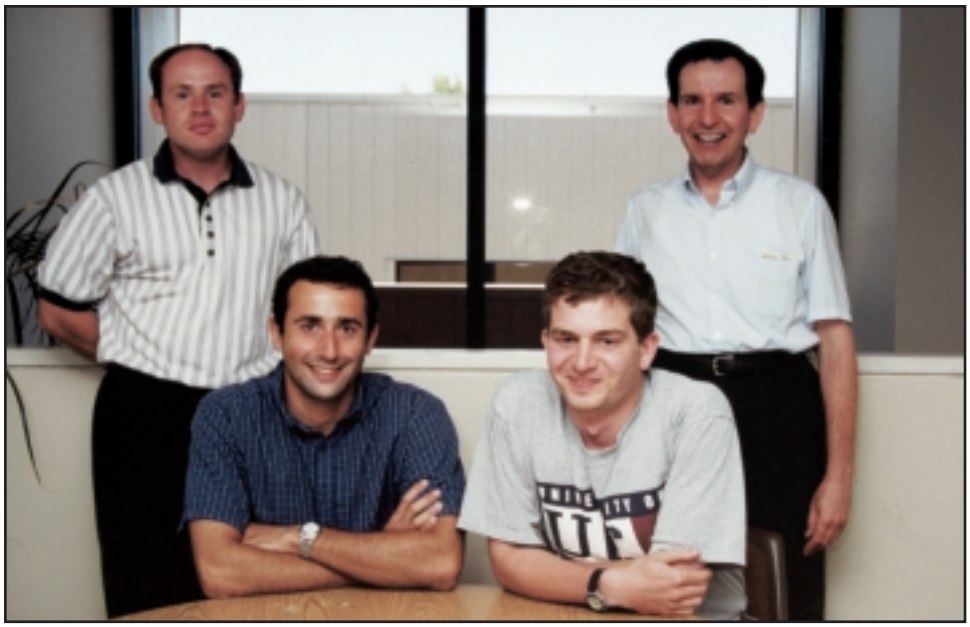
Figure 2. Planar LIF images of gasoline injected in the spark-ignited direct-injected experimental engine shown in Figure 1 reveal the effect of ambient cylinder pressure and fuel temperature on spray morphology. Annotations on the bottom of each image indicate fuel temperature and ambient cylinder pressure at the start of injection. All images are recorded 1.3 ms into a 1.5-ms injection with a fuel pressure of 8 MPa while motoring at 1300 rpm. Increasing liquid fuel concentration is shown by the progression of colors from blue to green to yellow to red to white.

People

Eric Stevens has been a postdoctoral researcher working with Dick Steeper in the spark-ignition direct-injection laboratory. He has taken a position at General Electric Aircraft engines in Cincinnati, Ohio.



Visiting scientists Peter L. Kelly-Zion (left) and Dale Tree (right) have been working with John Dec in the Heavy-Duty Diesel Engine Laboratory. Peter, a professor at Trinity University in San Antonio, Texas, returned to the CRF for a month and a half this summer to continue investigations into the sources of diesel-engine soot emissions that he started during a postdoctoral stay with John between 1998 and 1999. Dale, who is a professor at Brigham Young University in Provo, Utah, has spent a sabbatical year with John working on several projects, including an investigation of diffusion-flame/wall interactions in the diesel engine and a related investigation of soot deposition rates on the combustion chamber wall. Both visitors worked on the Sandia/Cummins optically accessible diesel engine visible between Peter and John.



As part of their ongoing collaborative work with a DOE-supported computational modeling program at the University of Chicago, CRF staffers (standing, left to right) Scott Wunsch and Alan Kerstein hosted visiting Chicago graduate students (seated, left to right) Adam Oberman and Jonathan Dursi this summer. Adam and Jonathan performed computational studies of turbulent mixing and combustion phenomena related to astrophysical explosions.

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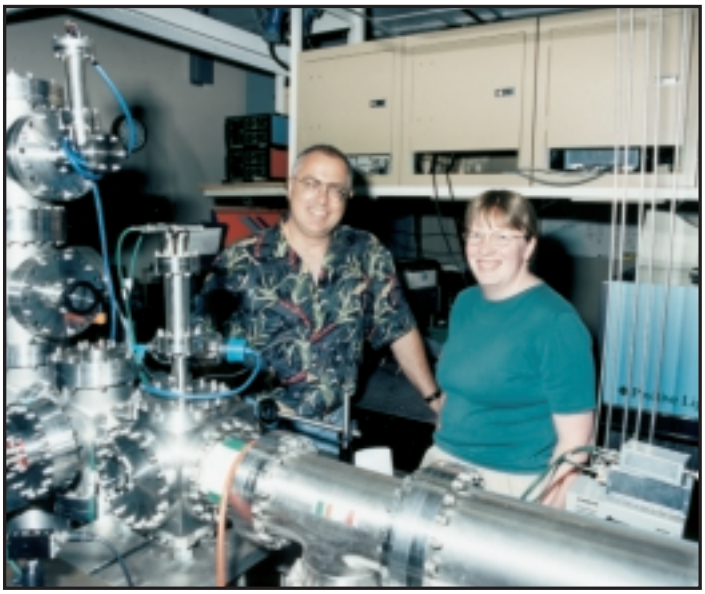

Postdoctoral researcher Elisabeth Wade and Dave Chandler stand behind the crossed molecular-beam ion-imaging apparatus that Elisabeth has used for the past year to study rotationally inelastic bimolecular collisions. Elisabeth has accepted a position as Assistant Professor of Chemistry at Mills College in Oakland California.

Stephen Klippenstein (left), who recently joined the Combustion Chemistry Department, discusses his work with new Department Manager John Goldsmith. Stephen was a two-time visiting researcher from 1998 to the time of his hire, and John returns to the CRF after an absence of 4 years.

Events

CRF Scientists Present Papers in Scotland

The CRF was well represented at the 28th International Symposium on Combustion held at the University of Edinburgh from July 30 to August 4. Sandia researchers coauthored 26 papers and posters that were presented at the weeklong symposium. Jim Miller, Rob Barlow, Jackie Chen, and Don Hardesty chaired colloquia and technical sessions.

Oral Presentations:

Stretch Effects on the Burning Velocity of Turbulent Premixed Hydrogen-Air Flames, Jackie Chen and Hong Im of the University of Michigan.

Effects of Flow Transients on the Burning of Velocity of Laminar Hydrogen-Air Premixed Flames, Jackie Chen and Hong Im of the University of Michigan.

Modeling of On-Line Catalyst Addition Effects in a Short Contact Time Reactor, Mark Allendorf, David Zerkle of Los Alamos National Laboratory, and Markus Wolf and Olaf Deutschmann of the University of Heidelberg.

Radiation and Nitric Oxide Formation in Turbulent Non-Premixed Jet Flames, Jonathon Frank, Rob Barlow, and C. Lundquist.

A Shutter-Based Line-Imaging System for Single-Shot Raman Scattering Measurements, Rob Barlow and Paul Miles.

A Computational Study of the Effect of Fuel-Type on Ignition Time in HCCI Engines, John Dec and Peter Kelly-Zion of Trinity University.

Scaling and Efficiency of PRISM in Adaptive Simulations of Turbulent Premixed Flames, Joe Grcar and John Bell, Nancy Brown, Marcus Day, Michael Frenklach, Richard Propp, and Shaheen Tonse of Lawrence Berkeley National Laboratory.

A Laser and Molecular Beam Mass Spectrometer Study of Low-Pressure Dimethyl Ether Flames, Andy McIlroy, Toby Hain, and Hope Michelsen and Terry Cool of Cornell University.

A Theoretical Analysis of the Reaction Between Ethyl and Molecular Oxygen, Jim Miller and Stephen Klippenstein of Case Western Reserve University and Struan Robertson of Molecular Simulations, Inc.

Exploring Old and New Benzene Formation Pathways in Low-Pressure Premixed Flames of Aliphatic Fuels, Chris Pope and Jim Miller.

Triple Flame Structure and Dynamics at the Stabilization Point of an Unsteady Lifted Jet Diffusion Flame, Habib Najm, J. Ray, K. D. Devine, and S. Kempka and R. B. Milne of Xilinx Corp

Dynamic Response of Strained Premixed Flames to Equivalence Ration Gradients, Habib Najm and Y. M. Marzouk and A. F. Ghonium of the Massachusetts Institute of Technology.

Reaction Rate Imaging, Jason Rehm and Phil Paul

Effect of Stoichiometry and Strain-Rate on Transient Flame Response, Habib Najm and Omar Knio of The Johns Hopkins University.

The Dependence of Chemistry on the Inlet Equivalence Ratio in Vortex-Flame Interactions, Joe Grcar and John Bell, Nancy Brown, Marcus Day, Michael Frenklach, and Shaheen Tonse of LBNL

CRF Hosts Particulate Matter Workshop

The Combustion Research Facility and the U.S. Department of Energy hosted a workshop entitled, "Particulate Matter from Reciprocating Engines: Diagnostic Needs." It was organized by Bob Carling, Simone Hochgreb, and Pete Witze. The workshop brought together experts from industry, academia, and research institutions to review current research, future diagnostic needs, and ways to leverage resources. About 50 people participated representing 29 organizations.

Three Distinct Temperature Regimes Predicted for the Kinetics of Ethyl Oxidation by Molecular Oxygen

Jim Miller and Stephen Klippenstein, in collaboration with Struan Robertson of Molecular Simulations, Inc. of Cambridge, England, have completed an extensive theoretical investigation of the reaction between ethyl (C_2H_5) and molecular oxygen. This reaction is commonly viewed as prototypical of R(alkyl) + O_2 reactions in general, whose behavior is responsible for the "negative temperature coefficient" regime in the oxidation of alkanes. The analysis consisted of using a combination of electronic-structure theory (both a G2-like approach and the B3LYP density functional method), variational transition-state theory to calculate RRKM rate coefficients, and solving the time-dependent, chemically activated master equation to characterize the rate and product distribution over wide ranges of temperature and pressure. Figure 1 shows the reaction path diagram on which the analysis was based. In agreement with Fritz Schaefer and coworkers at the University of Georgia, the diagram shows that C_2H_4 + HO_2 is formed by direct elimination from the ethylperoxy adduct.

The most interesting and important result of the analysis is the prediction of three distinct temperature regimes for the kinetics, shown in Figure 2. At low temperature (T < 575 K), everything behaves normally, i.e. the deficient reactant (C_2H_5) decays exponentially, and the products ($C_2H_5O_2$ or C_2H_4 + HO_2) are functions of temperature and pressure. The transition regime (575 K < T < 700 K) is characterized by biexponential decays of C_2H_5 and a rapid increase in the production of bimolecular products (C_2H_4 + HO_2) with temperature as the rate coefficient drops (corresponding to equilibration of the stabilization reaction). As Figure 2 shows, at high temperature (T > 700 K), the reaction $C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$ can be written as an elementary step whose rate coefficient is independent of pressure. These predictions agree well with the experimental results of Wagner et al. (1990), Kaiser et al. (1990, 1995), and Slagle et al.(1990)

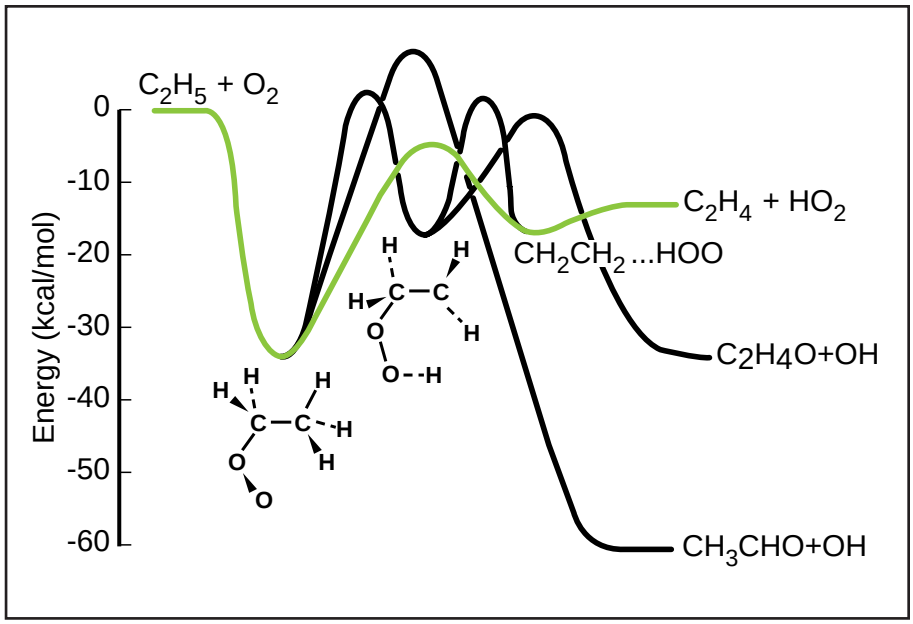

Figure 1. Reaction path diagram of the reaction of ethyl with molecular oxygen showing the most likely reaction path (green line). Calculations predict that over 90% of the reaction proceeds along this pathway, even at T=2000K. Bond energies of stable intermediates and transition states were determined from G2-like, B3LYP, and master equation calculations.

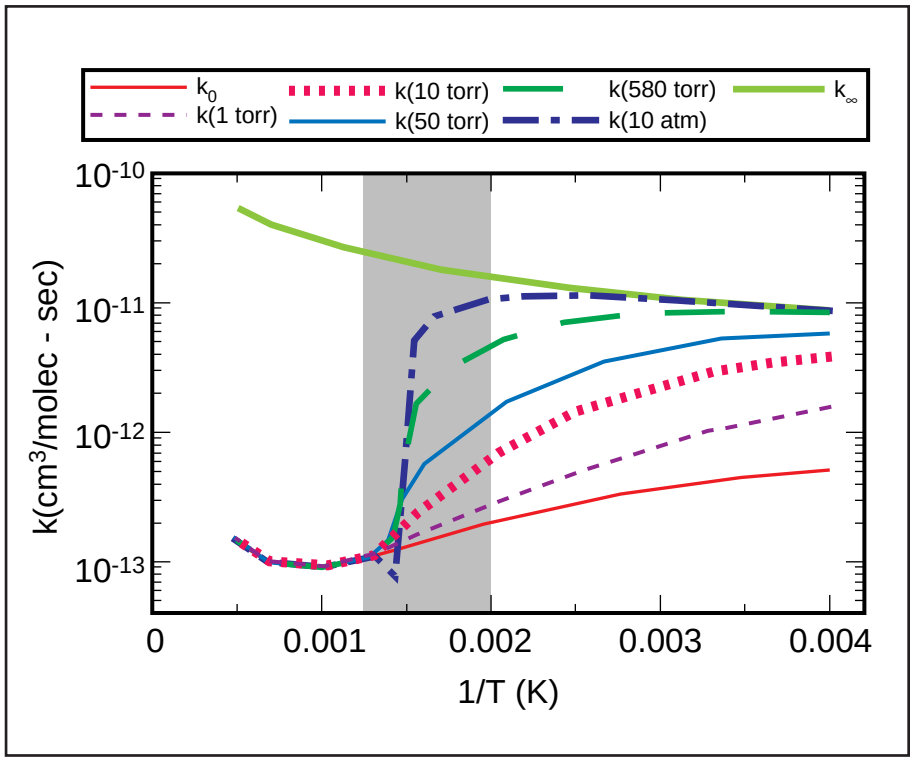

Figure 2. Plots of rate coefficients versus temperature for a series of pressures for the reaction of ethyl with oxygen. The plots show that as temperature increases (right to left) the reaction kinetics go through three distinct temperature regimes. Kinetics are normal at low temperatures, complex (nonexponential reactant decays) in the transition regime (the shaded area in the figure), and independent of pressure in the high temperature regime.

Simulation of Oceanic Turbulence Aids Combustion Modeling

Improvements in the predictive capability of turbulent combustion models will require accurate representation of turbulence interactions with molecular transport processes in flames. To achieve the needed improvements, Sandia researchers are investigating other flows in which the interplay between turbulence and molecular transport is important.

A dramatic example of this interplay is the spontaneous formation of layers in stably stratified fluid that is continually stirred to generate turbulence. This self-organization into well-mixed turbulent regions separated by narrow interfaces with steep property gradients has been demonstrated in laboratory experiments, and it may account for structure observed in oceans.

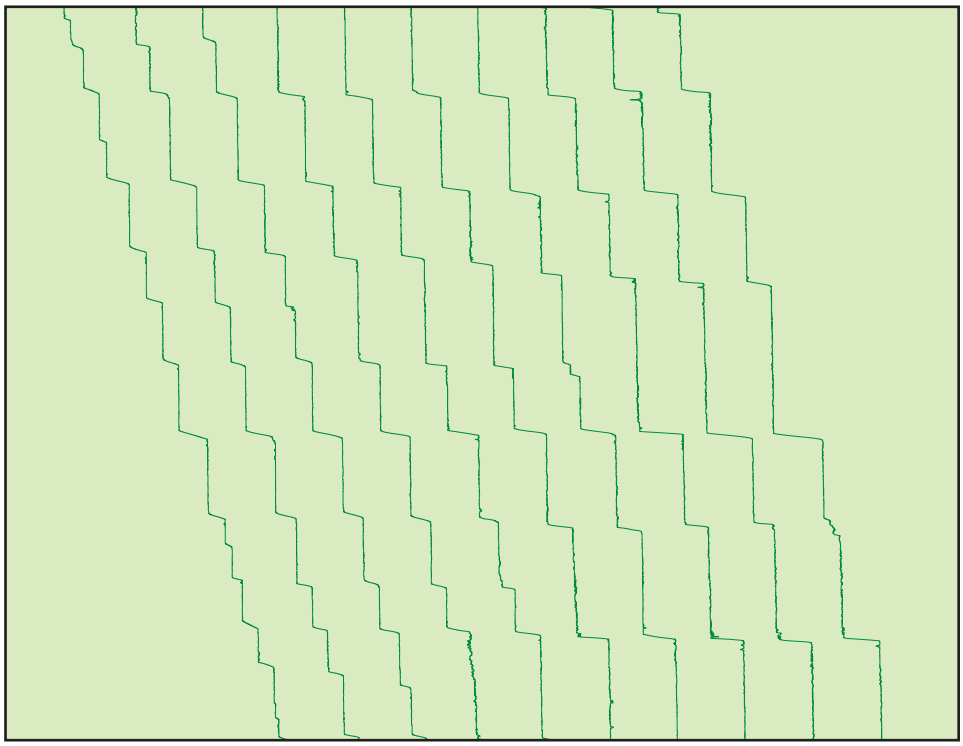

Figure 1. Simulated vertical profiles of density as a function of depth in a turbulent fluid with a linear initial density profile. The steps in each profile represent the boundaries between layers of different density. The series of profiles, which represent increasing time from left to right, shows that small layers form, merge, and eventually stabilize when the energy barriers between layers become sufficiently high to suppress penetration of the layers by turbulence.

Sandia researchers Alan Kerstein and Scott Wunsch have simulated the layered state numerically and have analyzed its structure from the viewpoint of turbulence interaction with molecular transport in the high-gradient regions. A one-dimensional statistical model, denoted One-Dimensional Turbulence, was used to perform the simulations because the wide range of length scales seen in the profiles cannot be resolved affordably in a multidimensional simulation. The simulations capture the influence of molecular transport processes in the sharp interfaces on larger scale processes that determine layer width.

Based on reasoning analogous to turbulent combustion theory, Alan and Scott obtained predictions that are supported by laboratory experiments and their computer simulations. This outcome will promote further development of improved turbulent combustion models. Despite this progress, there is not yet a fundamental understanding of the cause of layering.

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